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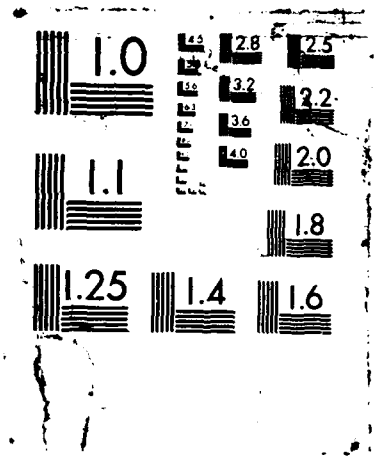
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4. PERFORMING ORGANIZATION REPORT NUMBER(S)	5. MONITORING ORGANIZATION REPORT NUMBER(S): AFOSR-TR- 87-1983
6a. NAME OF PERFORMING ORGANIZATION: Inst. for Scientific Computing; 6b. OFFICE SYMBOL (If applicable)	7a. NAME OF MONITORING ORGANIZATION: AFOSR/NM
6c. ADDRESS (City, State, and ZIP Code): P.O. Box 1388, Fort Collins, Colorado 80522	7b. ADDRESS (City, State, and ZIP Code): AFOSR/NM, Bldg 410, Bolling AFB DC 20332-6448
8a. NAME OF FUNDING/SPONSORING ORGANIZATION: AFOSR; 8b. OFFICE SYMBOL (If applicable): NM	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER: AFOSR-87-0133
8c. ADDRESS (City, State, and ZIP Code): AFOSR/NM, Bldg 410, Bolling AFB DC 20332-6448	10. SOURCE OF FUNDING NUMBERS: PROGRAM ELEMENT NO. 61102F; PROJECT NO. 2304; TASK NO. A3; WORK UNIT ACCESSION NO.

11. TITLE (Include Security Classification)

Fast Algorithms for Euler and Navier-Stokes Simulations

12. PERSONAL AUTHOR(S)

Professor Johnson

13a. TYPE OF REPORT	13b. TIME COVERED	14. DATE OF REPORT (Year, Month, Day)	15. PAGE COUNT
Final	FROM 1/1/87 TO 9/30/87	Nov. 30,1987	12

16. SUPPLEMENTARY NOTATION

17. COSATI CODES			18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)
FIELD	GROUP	SUB-GROUP	

19. ABSTRACT (Continue on reverse if necessary and identify by block number)

An explicit flow solver, applicable to the hierarchy of model equations ranging from Euler to full Navier-Stokes, was combined with several techniques designed to reduce computational expense. The computational domain consisted of local grid refinements embedded in a global coarse mesh, where the locations of these refinements are defined by the physics of the flow. Flow characteristics were also used to determine which set of model equations is appropriate for solution in each region, thereby reducing not only the number of grid points at which the solution must be obtained, but also the computational effort required to get that solution. Acceleration to steady-state was achieved by applying multigrid on each of the subgrids, regardless of the particular model equations being solved. Since each of these components is explicit, advantage could readily be taken of the vector-and parallel-processing capabilities of machines such as the Cray X-MP and Cray 2.

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Air Force Office of Scientific Research
Grant 87-0133

Fast Algorithms for Euler and Navier-Stokes Simulations

Final Technical Report

30 November 1987

Institute for Scientific Computing
P.O. Box 1988
Fort Collins, Colorado 80522

Summary

An explicit flow solver, applicable to the hierarchy of model equations ranging from Euler to full Navier-Stokes, is combined with several techniques designed to reduce computational expense. The computational domain consists of local grid refinements embedded in a global coarse mesh, where the locations of these refinements are defined by the physics of the flow. Flow characteristics are also used to determine which set of model equations is appropriate for solution in each region, thereby reducing not only the number of grid points at which the solution must be obtained, but also the computational effort required to get that solution. Acceleration to steady-state is achieved by applying multigrid on each of the subgrids, regardless of the particular model equations being solved. Since each of these components is explicit, advantage can readily be taken of the vector- and parallel-processing capabilities of machines such as the Cray X-MP and Cray-2.

1. Introduction

It is generally recognized that a comprehensive approach to the simulation of flows involving both complex geometries and complex physics will require powerful advanced-architecture supercomputers with very large memories. Machines capable of producing solutions to Reynolds-averaged Navier-Stokes flows over complex geometries within computing times short enough to be of design interest are expected to be available by the end of this decade [1]. In order to use these parallel-processing supercomputers effectively, algorithms must be adapted to focus the power of multiple processing units on a single flow simulation. Furthermore, the history of computational aerodynamics teaches that the pace of progress in this field is set by the synergism between improved computers and better algorithms. In the past 15 years, improved computers have reduced the cost of computation by a factor of about 100. Over the same period, better algorithms have reduced the cost of computation on a given computer by a factor of almost 1000 [2]. Thus, it is to be expected that the need for faster algorithms will not be diminished by the availability of faster and larger computers.

The most popular algorithms presently in use for calculating three-dimensional Navier-Stokes flows are Beam-Warming [3] (or similar implicit methods) and two types of explicit schemes, Runge-Kutta [4] and Lax-Wendroff [5]. Implicit schemes are highly efficient on uniprocessor machines, and may even be adapted to parallel computers with a small number of processors and shared memory [6]. However, as shown by Bruno [7], they are extremely sensitive to the size and location of memory in large multiprocessor systems. Runge-Kutta and Lax-Wendroff methods, on the other hand, being explicit, map readily onto parallel architectures. The authors chose to use MacCormack's method in the present work because of its robustness and their experience with it, although another explicit scheme, such as Runge-Kutta, could be used in its place. The approach selected enhances the efficiency of the MacCormack scheme by implementing it on a collection of local meshes embedded in a global mesh. Either the Euler, thin-layer Navier-Stokes or full Navier-Stokes equations are solved on designated meshes. The choice of model equations is determined by the nature of the flow physics to be resolved on a particular mesh. When the requirement for time accuracy is relaxed, a convergence acceleration procedure is applied simultaneously to all meshes and all model equations. The entire algorithm is explicit and is designed to perform well on computers consisting of multiple processing units, each having vector processing capability. Examples of such machines are the Cray X-MP and Cray 2.

All of the above-mentioned elements of the algorithm have been integrated into a fully three-dimensional Navier-Stokes flow solver, the performance of which is being evaluated. This task requires a very large memory, high-speed computer such as the Cray-2. It has 256 million words of shared memory and four vector CPUs and is the principal machine being used for development and testing of the scheme. However, until mature, reliable multitasking software is available on the Cray-2, this aspect of the development will be continued on the X-MP, which is also a four-processor system. Since the X-MP presently has at most 16 million words of primary memory, the problem has to be scaled back by decreasing the number of grid points. It is conjectured that parallel-processing efficiency degrades for smaller problems, so that the X-MP will provide a lower bound on expected performance of the full-scale simulation.

2. Equations of Motion

The nondimensional equations of motion may be written in conservation-law form as

$$q_t = -(F_x + G_y + H_z)$$

where, for the Reynolds-averaged Navier-Stokes equations,

$$F = f - Re^{-1}p \qquad G = g - Re^{-1}r \qquad H = h - Re^{-1}s$$

while, for their thin-layer version,

$$F = f \qquad G = g \qquad H = h - Re^{-1}d$$

and, for the Euler equations,

$$F = f \qquad G = g \qquad H = h$$

where:

$$q = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ E \end{bmatrix} \qquad f = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ \rho uw \\ (E+p)u \end{bmatrix} \qquad g = \begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ \rho wv \\ (E+p)v \end{bmatrix}$$

$$h = \begin{bmatrix} \rho w \\ \rho uw \\ \rho vw \\ \rho w^2 + p \\ (E+p)w \end{bmatrix} \qquad d = \begin{bmatrix} 0 \\ \mu u_z \\ \mu v_z \\ (\lambda+2\mu)w_z \\ \gamma\kappa Pr^{-1}e_z + (\lambda+2\mu)ww_z \end{bmatrix}$$

$$p = \begin{bmatrix} 0 \\ \tau_{xz} \\ \tau_{yz} \\ \tau_{zz} \\ \beta_z \end{bmatrix} \qquad r = \begin{bmatrix} 0 \\ \tau_{xy} \\ \tau_{yy} \\ \tau_{zy} \\ \beta_y \end{bmatrix} \qquad s = \begin{bmatrix} 0 \\ \tau_{xz} \\ \tau_{yz} \\ \tau_{zz} \\ \beta_z \end{bmatrix}$$

$$\tau_{xx} = \lambda(u_x + v_y + w_z) + 2\mu u_x \qquad \beta_x = \gamma\kappa Pr^{-1}e_x + u\tau_{xx} + v\tau_{xy} + w\tau_{xz}$$

$$\tau_{yy} = \lambda(u_x + v_y + w_z) + 2\mu v_y \qquad \beta_y = \gamma\kappa Pr^{-1}e_y + u\tau_{yx} + v\tau_{yy} + w\tau_{yz}$$

$$\tau_{zz} = \lambda(u_x + v_y + w_z) + 2\mu w_z \qquad \beta_z = \gamma\kappa Pr^{-1}e_z + u\tau_{zx} + v\tau_{zy} + w\tau_{zz}$$

$$\tau_{xy} = \tau_{yx} = \mu(u_y + v_x), \quad \tau_{xz} = \tau_{zx} = \mu(u_z + w_x), \quad \tau_{yz} = \tau_{zy} = \mu(v_z + w_y)$$

Here ρ, u, v, w, p and E are respectively density, velocity components in the x-, y- and z-directions, pressure and total energy per unit volume. This final quantity may be expressed as

$$E = \rho\left(e + \frac{1}{2}(u^2 + v^2 + w^2)\right)$$

where the specific internal energy, e, is related to the pressure and density by the simple law of a calorically-perfect gas

$$p = (\gamma - 1)\rho e$$

with γ denoting the ratio of specific heats. The coefficient of thermal conductivity, κ, and the viscosity coefficients, λ and μ, are assumed to be functions only of temperature. Furthermore, λ is expressed in terms of the dynamic viscosity, μ, by invoking Stokes' assumption of zero bulk viscosity. Re and Pr denote the Reynolds and Prandtl numbers, respectively. Although, for simplicity, the equations of motion are presented here written in Cartesian coordinates, it is well known that their strong conservation law form may be maintained under an arbitrary space- and time-dependent transformation of coordinates.

3. Algorithm Strategy

In order to minimize the cost of simulating complex, three-dimensional viscous flow over complete configurations, the following strategy has been developed:

a. Use a robust and flexible explicit flow solver capable of simulating either steady or unsteady flow with the Euler, thin-layer Navier-Stokes or full Navier-Stokes equations.
b. Distribute grid points optimally by making use of both grid stretching and locally-embedded grid refinements.
c. Make use of a zonal flow simulation strategy ranging from the Euler equations through the full Navier-Stokes equations in order to minimize the computational work per grid point.
d. Accelerate the convergence of steady flow simulations by means of an explicit multigrid technique which may be applied, without modification, to the entire hierarchy of model equations. Use additional convergence acceleration methods, such as residual averaging, as appropriate.
e. Take advantage of the explicit nature of the algorithm by mapping it onto a supercomputer architecture consisting of multiple vector-processing CPUs and thus enhance its performance by means of both vectorization and multitasking.

Further detail concerning this strategy is provided in [8].

4. Parallel Processing Considerations

Parallel processing may be viewed in terms of a collection of separately-running programs, called processes, which exchange information among themselves by means of some interconnection scheme. The effects of load balancing, granularity, overhead, and Amdahl's law are all important factors affecting the performance of parallel computers.

Amdahl's law [9] points out that if a computer has two speeds of operation, the slower mode will dominate performance as the faster mode becomes arbitrarily fast. This can be expressed by the relation

$$S = (R + (1 - R) / N)^{-1}$$

where S is the maximum speedup achievable by using N processors on an application which has a fraction of code, R, which must be executed in sequential mode. For example, if R is assumed to be .02, the maximum speedup attainable on a four-processor machine will be 3.77.

The effects on speedup of granularity and overhead, which are also important considerations in multitasking, may be illustrated as follows:

$$S = G\,(\,O + G\,/\,N\,)^{-1}$$

Granularity, G, is defined as the length of time required to execute some code segment on a single processor. Although smaller-grained tasks are generally easier to create than larger ones, the overhead, O, associated with creation, synchronization, etc., may negate any performance gains which would otherwise result from parallel execution of smaller tasks. To attain a speedup of 3.77 using four processors would, for example, require that the granularity be more than 65 times the overhead.

A third concern in multitasking is load balancing, or the distribution of computational work across some number of processors. Static and dynamic partitioning may be employed to try to keep all processors equally busy. Static partitioning is most effective when tasks of equal work can be defined *a priori*; dynamic partitioning may enable better load balancing for tasks of varying length, if the additional synchronization overhead incurred is not too great.

Extensions to programming languages which allow the creation and termination of processes, synchronization of processes, and communication among them are necessary for multiprocessing. Both the Cray-2 and the Cray X-MP have software libraries that provide such multitasking tools. Two variations of multitasking are available on the X-MP, namely, macrotasking and microtasking. Macrotasking is intended for application to large-grained problem partitioning, while microtasking, by virtue of its very low overhead, may be used efficiently at a fine-grained level. Only macrotasking is available on the Cray-2. For the current application, both types of multitasking have been examined and tested. Microtasking is easily implemented in a code which has been optimized for vectorization. Macrotasking, however, requires careful examination of the problem in order to define large code structures for parallel execution. More detailed discussions of these multitasking concepts and others may be found in Larson [10], Johnson [11], and Misegades et al. [12].

5. Test Problem

The geometry of the three-dimensional model problem is representative of a turbomachinery application and consists of a rectilinear cascade of finite-span, swept blades mounted between endwalls. Test cases include inviscid subsonic flows and transonic flows with shocks, and viscous laminar and turbulent flows for Reynolds numbers ranging from 8.4×10^3 to 2.0×10^5 (based on cascade gap and critical speed). We believe internal flow problems to be more challenging than external problems for a number of reasons. These include the fact that internal problems limit one's ability to use grid stretching, and that lateral solid boundaries slow convergence by only letting transients propagate out the inlet and exit rather than radiating to infinity in all directions.

The computational domain is partitioned by the collection of embedded meshes. Three levels of grid fineness are used in the present application. If the coarsest mesh (grid 3) is thought of as covering the whole domain, the embedded meshes are then formed by halving or quartering the grid spacing in selected regions. Grid 1 refers to the finest mesh, which lies along the juncture between the blade and the endwalls. Grid 2, coarser than grid 1 by a factor of two, encompasses all surfaces not in grid 1, i.e., the blade and wall surfaces away from the corners. Any coarse-grid points underlying the finer grids are coincident with points on those grids. The intergrid boundaries are treated by overlapping the grids such that the boundary of an embedded mesh lies on the interior of one of its neighboring meshes, with interpolation used where necessary to fill in the surfaces.

When the set of three grids described above is used, the full Navier-Stokes equations are solved on mesh 1, the thin-layer Navier-Stokes equations are solved on mesh 2 and the Euler equations are solved on the coarsest mesh, mesh 3. The flowfield updating begins with mesh 1. After one timestep on mesh 1, mesh 2 is updated exterior to mesh 1 while convergence acceleration is applied at the mesh-2 points interior to mesh 1. Next, mesh 3 is updated exterior to mesh 2 while convergence acceleration is applied at the mesh-3 points interior to mesh 2. Updating proceeds in this fashion until the global mesh has been advanced by one timestep. Then the updating cycle is completed by applying convergence acceleration to coarsenings of the global grid. This cycle is repeated until the desired measure of convergence is satisfied.

6. Performance Evaluation

Performance of parallel computers is evaluated by comparing wall clock time for both uniprocessed and multiprocessed runs on a dedicated machine. This ratio is called the speedup. Dividing the speedup by the number of processors gives the efficiency of processor utilization, a measure of load balancing and overhead.

A two-dimensional version of the code makes extensive use of parallelism inherent in the physical problem to obtain a good load balance when using the X-MP macrotasking software. As the macrotasking approach requires the use of calls to a subroutine library, it has rather high overhead and thus yields best results for large-grained code segments. Table I presents some two-dimensional macrotasking results from both a Cray X-MP/48 and a Cray-2, for the basic solver with multigrid. X-MP performance shows that the algorithm has been efficiency parallelized, while the poorer performance on the Cray-2 is due to less mature macrotasking software on that machine. In Table II, macrotasking results for the basic solver are shown and contrasted with the same code run using the microtasking approach. Microtasking is managed within CPUs, through the use of the X-MP cluster registers. The very low overhead attained by microtasking allows users to partition code at a fine-grained level while still making efficient use of two or more CPUs. The microtasking results in Table II are only marginally better than the macrotasking ones because the algorithm employed in the test had been restructured to maximize task granularity. Three-dimensional microtasking results for a small-grained partitioning of the algorithm are shown in Table III.

Comparison of the embedded-mesh algorithm with a single-mesh algorithm yields the following general conclusion: the accuracy of the embedded-mesh results is essentially that of a global finest mesh, while the convergence rate is like that of a global coarsest mesh. In two-dimensional computations, using the Euler and thin-layer Navier-Stokes equations and three mesh regions, embedding speedups as high as 30 in comparison to a single-mesh algorithm have been obtained (see Table IV). A three-dimensional algorithm has been designed and implemented. As shown in Table V, results have been obtained for simple embeddings which span the y direction, using relatively coarse grids with no tuning. These results are consistent with their two-dimensional analogs.

7. Conclusions

A procedure for solving complex three-dimensional aerodynamic flows on parallel-processing supercomputers has been presented. This procedure incorporates a number of innovations in order to attain high levels of computational efficiency. These innovations include: locally-embedded mesh refinements, a zonal flow simulation strategy that solves the Euler equations through the full Navier-Stokes equations, multigrid convergence acceleration applied to a robust explicit basic flow solver, and both vectorization and multitasking.

Computations have been carried out on parallel-processing supercomputers, principally on the Cray-2, but also on the Cray X-MP because of its more sophisticated multitasking software. The results presented here illustrate that a four CPU shared-memory multiprocessor can be used to carry out aerodynamics simulations with a high degree of efficiency.

The embedded grid scheme has demonstrated performance increases on the order of 30 compared to the global fine grid solution, while maintaining the fine grid solution accuracy.

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Tables

Table I. Two-Dimensional Macrotasked Multigridded Scheme Performance

Machine	2 Processors		4 Processors	
	Speedup	Efficiency	Speedup	Efficiency
Cray X-MP	1.87	0.94	3.30	0.83
Cray 2	1.80	0.90	2.58	0.65

Table II. Two-Dimensional Multitasked Basic Solver Performance

Machine	2 Processors		4 Processors	
	Speedup	Efficiency	Speedup	Efficiency
Cray X-MP with macrotasking	1.91	0.96	3.58	0.90
Cray X-MP with microtasking	1.93	0.97	3.78	0.95

Table III. Three-Dimensional Microtasked Multigridded Scheme Performance

Machine	2 Processors		3 Processors		4 Processors	
	Speedup	Efficiency	Speedup	Efficiency	Speedup	Efficiency
Cray X-MP	1.96	0.98	2.83	0.94	3.55	0.89

Table IV. Two-Dimensional Embedding Speedups
(129 x 33 x 33 finest grid, 2 embeddings)

Test Case	Speedup
Inviscid Subcritical	16.4
Inviscid Supercritical	6.1
Turbulent Viscous	30.2

Table V. Three-Dimensional Embedding Speedups
(65 x 17 x 17 finest grid, 1 embedding)

Test Case	Speedup
Inviscid Subcritical	7.0
Inviscid Supercritical	4.6
Turbulent Viscous	16.0

END

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